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Theoretical prediction of a novel class of electrides for applications in redox catalysis and quantum computing

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This high-level quantum chemical study reveals that metal complexes can accommodate bound diffuse electrons in their periphery making species, which mimic hydrogenic atoms. These complexes (called solvated electron precursors or SEPs) are present in concentrated metal ammonia solutions, where solvated electrons orbit around the positively charged metal ammonia skeleton. A typical example is Li (NH3)4, which has a Li (NH3)4^+ core and one peripheral electron populating a hydrogenic shell model but with the nuclear or jellium shell energy order: 1s, 1p, 1d, 2s, 2p, 1f, 2d. We demonstrate that transition metal ammonia complexes retain electrons in both their inner-d shell and the peripheral orbitals. In addition, two such complexes can bind together (like two hydrogen atoms producing molecular hydrogen) and form σ, σ*, π, π* orbitals identical to traditional diatomic molecules. The formation of dimers and polymers is confirmed experimentally in saturated lithium ammonia solutions, which create the so-called liquid or expanded metals. For the first time, we propose novel materials by either bridging of two SEPs with diamines or anchoring SEPs on appropriate surfaces. We demonstrate that such materials can capture, reduce, and convert CO2 to industrial platform chemicals and that the spin of the diffuse electrons can serve as a high-quality qubit. Based on these results, we proposed the existence of novel 2d- and 3d-materials composed of linked-SEPs, which can serve both as redox catalysts and quantum computing materials.

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